

THE ROTATIONAL SPECTRA OF IO AND BrO

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IO^a and BrO^b were among the first highly reactive free radicals to be studied by microwave spectroscopy. Although there have been subsequent investigations of the spectra of both molecules, high resolution data for the upper vibrational states ($v > 2$) of the $X_1^2\Pi_{3/2}$ states have remained sparse. The only high resolution work on the $X_2^2\Pi_{1/2}$ state of either molecule is the X_1 - X_2 LMR study of McKellar.^c Because of their possible role in processes affecting upper atmospheric chemistry, we have re-examined the rotational spectra of these molecules under conditions which populate the more highly excited states.

The rotational spectra of IO in vibrational states up to $v = 13$ in the $X_1^2\Pi_{3/2}$ state and up to $v = 9$ in the $X_2^2\Pi_{1/2}$ state have been observed in an O₂ DC discharge over molecular I₂. In addition, I¹⁸O has been observed for both the X_1 and X_2 states up to $v = 5$. This provides the first rotational data for the X_2 state and for I¹⁸O. All data have been analyzed simultaneously with fixed isotopic ratios among the constants. Vibrationally hot BrO has also been observed in an O₂ DC discharge which contains a small amount of Br₂. The BrO measurements are still in progress and have been extended to $v = 6$ for the $X_1^2\Pi_{3/2}$ state and to $v = 3$ for the $X_2^2\Pi_{1/2}$ state of the ¹⁶O species. Br¹⁸O spectra for the vibrational ground state of both the X_1 and X_2 states as well as $v = 1$ of the X_1 state are included in a simultaneous fit of all four isotopomers. Extensive sets of parameters have been derived for both IO and BrO. These will be interpreted in terms of the electronic structure and the interatomic potential and compared with those of related molecules.

^aS. Saito, *J. Mol. Spectrosc.*, **48**, 530 (1973)

^bF. X. Powell and D. R. Johnson, *J. Chem. Phys.*, **50**, 4596 (1969)

^cA. R. W. McKellar, *J. Mol. Spectrosc.*, **86**, 43 (1981).